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Abstract (less than 300 words)

The paper will review the combined group contribution (GC) – atom connectivity (AC) approach for prediction of physical and thermodynamic properties of organic chemicals and their mixtures with special emphasis on lipids. This combined approach employs carefully selected datasets of different pure component properties to develop simultaneously two parallel models, one based on group contribution and another based on atom connectivity, for each property. The lipids present in the database are regarded as a separate class, for which special models for temperature dependent pure component properties have been implemented. For mixtures, properties related to phase equilibria are modelled with molecular models (UNIQUAC, NRTL) as well as the combined GC-AC approach. The collected phase equilibrium data for VLE. For SLE and LLE data, due to lack of established methods, consistency tests have not been performed. After the regression step, the stored regression statistical data is employed to calculate the covariance matrix and from it, the uncertainty of the predicted property value. The paper will also review the role of the databases and the mathematical and thermodynamic consistency of the measured/estimated data, the predictive nature of the developed models and the uncertainty estimates of the predicted data. Related to the database, the consistency of the collected data, the uncertainties in the measured values, and the amount of data to be used in the regression step, will be discussed and analyzed with respect to lipids and compared with the general trends involving the other organic chemicals in the database. Related to modelling, the predictive nature of the models, the calculation of the uncertainties of the estimated property values, the theoretical trends will be illustrated with examples involving lipids.